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MOLECULAR INTERACTION STUDY OF N-PHENYL MALEANILIC ACID AND N-PHENYL MALEIMIDE IN AQUEOUS DIMETHYL SULPHOXIDE AT 298.15 AND 303.15 K

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Abstract

Density and viscosity of N-phenyl maleanilic acid and N-phenyl maleimide have been measured in 80% aqueous dimethyl sulphoxide at 298.15 and 303.15 K. Using this data, parameters including apparent molar volume, limiting apparent molar volume, semi-empirical parameter and Jones-Dole viscosity coefficients were calculated. From theses parameters, different types and extent of molecular interactions (solute-solute, solute-solvent and solvent-solvent) present in the solution were predicted.

Keywords: *N-phenyl maleanilic acid, density, dimethyl sulphoxide, apparent molar volume.*

Introduction:

Cyclic maleimide is a multifunctional heterocyclic moiety due to its applications in biology [1-3] and pharmacology [4-7]. Density, viscosity, apparent molar volume, molar volume at infinite dilution and Jones-Dole equation parameters 'A' and 'B' are very useful to know the type of molecular interactions present and to understand different biochemical aspects at the body temperature. The results were interpreted in terms of solute-solute, solute-solvent and solvent-solvent interactions in these systems. Dimethyl sulphoxide is an aprotic and strongly associated due to highly polar S=O group. The study of DMSO is important because of its application in medicine [8-9]. Density and viscosity of some 4-substituted N-phenyl maleimides in aqueous dimethyl sulphoxide have been studied at 308.15 K [10]. The literature survey made us to think and work on the study of molecular interactions present in N- phenyl maleanilic acid and N-phenyl maleimide.

Experimental:

N-phenyl maleanilic acid (a) and N-phenyl maleimide (b) were synthesized [11] and purified by recrystallization technique in the laboratory. Triple distilled water and analytical reagent grade dimethyl sulphoxide of minimum assay of 99.9% (SD Fine Chemicals) were used for preparation of solution in the range 0.002 M to 0.01 M at room temperature.

The bicapillary pycnometer and Ubbelohde viscometer was calibrated [12] using triple distilled water. The density and viscosity of distilled acetone and toluene were evaluated with respect to water. The desired temperature was maintained with the help of thermostatic water bath. The solution densities and viscosities were measured at 298.15 and 303.15 K. The flow time was recorded by using digital stop watch. The different concentrations of solution were prepared in 80 % aqueous dimethyl sulphoxide. Using the following equation apparent molar volumes, ϕ_v were obtained [13-14].

$$\phi_v = \frac{1000\ (\ \rho_0 - \rho\ )}{C\ \rho_0} + \frac{M2}{\rho_0}$$

Where, M_2, C, ρ_0 and ρ are the molar mass of solute, concentration (mol. L^{-1}) and densities of the solvent and the solution respectively.

The apparent molar volumes ϕ_v were plotted against the concentration as per the Masson's equation [15].

$$\phi_v = \phi o_v + S_v C^{1/2}$$

Where ϕo_v is the limiting apparent molar volume and S_v is semi empirical parameter or associated constant which depends on the nature of solvent, nature of solute and temperature. The viscosity data of N-phenyl maleanilic acid and maleimide was analysed using Jones-Dole equation [16].

$$\frac{\eta_r - 1}{C^{1/2}} = A + B\ C^{1/2}$$

Where, $\eta_r = \eta/\eta_o$ and η, η_o are viscosities of the solution and solvent respectively. C is the molar concentration. The linear plot for $(\eta_r\text{-}1)/C^{1/2}$ vs $C^{1/2}$ were obtained. The intercept (A) predicts the extent of solute-solute interaction and the slope (B) reflect the extent of solute-solvent interaction.

Results and Discussion:

Density, viscosity, apparent molar volume and relative viscosity of N-phenyl maleanilic acid and maleimide in 80 % aqueous DMSO solution at 298.15 and 303.15 K are given in Table 1. For both maleanilic acid (a) and maleimide (b), the density and apparent molar volume ϕ_v found to be increased with concentration. The negative values of apparent molar

volume indicate the electrostrictive solvation of solute. The more negative ϕ_v values in acid (a) are due to strong molecular association i.e. presence of electrostriction and hydrophilic interaction (solute solvent interactions). Figure 1 shows linear plots of ϕ_v vs $C^{1/2}$ of maleanilic acid and maleimide solution at 298.15 and 303.15 K respectively. Masson's parameter ϕo_v (limiting apparent molar volume) and S_v (semi empirical parameter) were obtained from linear plots are listed in Table 2. The negative values of ϕo_v indicate weak or absence of solute-solvent interactions. In other words hydrophobic-hydrophobic group interactions are present. The high positive value of S_v indicates the presence of strong solute-solute interactions. Maleanilic acid (a) has more solute-solute interactions than maleimide (b). The viscosities of solutions were found to be increased with concentration. Figure 2 shows variation of $(\eta_r-1)/C^{1/2}$ vs $C^{1/}2$ at 298.15 and 303.15 K. The viscosity coefficients 'A' and 'B' obtained from the graph are shown in table 2. Falkenhagen coefficient (A) represent the extent of solute-solute interactions and 'B' is Jones-Dole coefficient representing measure of order and disorder introduced by solute in solvent (solute-solvent interactions). Positive values of 'A' show the presence of strong solute-solute interactions while negative values of 'B' shows weak solute-solvent interactions at low temperature. The value of 'A' for acid (a) was high indicates the presence of stronger solute-solute interactions than that for maleimide.

TABLE 1: Densities (ρ) ($g.cm^{-3}$), apparent molar volumes ϕ_v ($cm^3.mol^{-1}$), viscosities (η) and relative viscosities (η_r) of N-phenyl maleanilic acid (a) and maleimide (b) in aqueous dimethyl sulphoxide at 298.15 and 303.15 K.

Comp.	Conc. (C) mol dm^{-3}	√C	Density (ρ) (g/cc)	ϕ_v (cm^3. mol^{-1})	Viscosity (η)	Relative viscosity (η_r)
298.15 K						
a	0.002	0.0447	1.09912	-1171.187	3.39660	1.02595
	0.004	0.0632	1.09929	-537.1612	3.40329	1.02797
	0.006	0.0775	1.09954	-337.9828	3.41638	1.03192
	0.008	0.0894	1.09991	-252.0776	3.42369	1.03413
	0.01	0.1	1.10042	-213.3063	3.43761	1.03833
b	0.002	0.0447	1.09822	-777.0966	3.35076	1.01210
	0.004	0.0632	1.09836	-341.4890	3.36349	1.01595
	0.006	0.0775	1.09858	-208.4500	3.37647	1.01987
	0.008	0.0894	1.09886	-148.7725	3.38349	1.02199
	0.01	0.1	1.09935	-132.1236	3.39116	1.02430
303.15 K						
a	0.002	0.0447	1.09689	-1118.6041	3.06405	1.02414
	0.004	0.0632	1.09699	-494.7809	3.07662	1.02834
	0.006	0.0775	1.09731	-320.3541	3.08366	1.03070
	0.008	0.0894	1.09763	-233.1407	3.09071	1.03305
	0.01	0.1	1.09815	-199.0932	3.10448	1.03766

b	0.002	0.0447	1.09601	-732.8939	3.02475	1.01101
	0.004	0.0632	1.09619	-328.4371	3.03139	1.01323
	0.006	0.0775	1.09641	-199.7117	3.04428	1.01754
	0.008	0.0894	1.09666	-138.7766	3.05112	1.01982
	0.01	0.1	1.09702	-112.2698	3.05827	1.02221

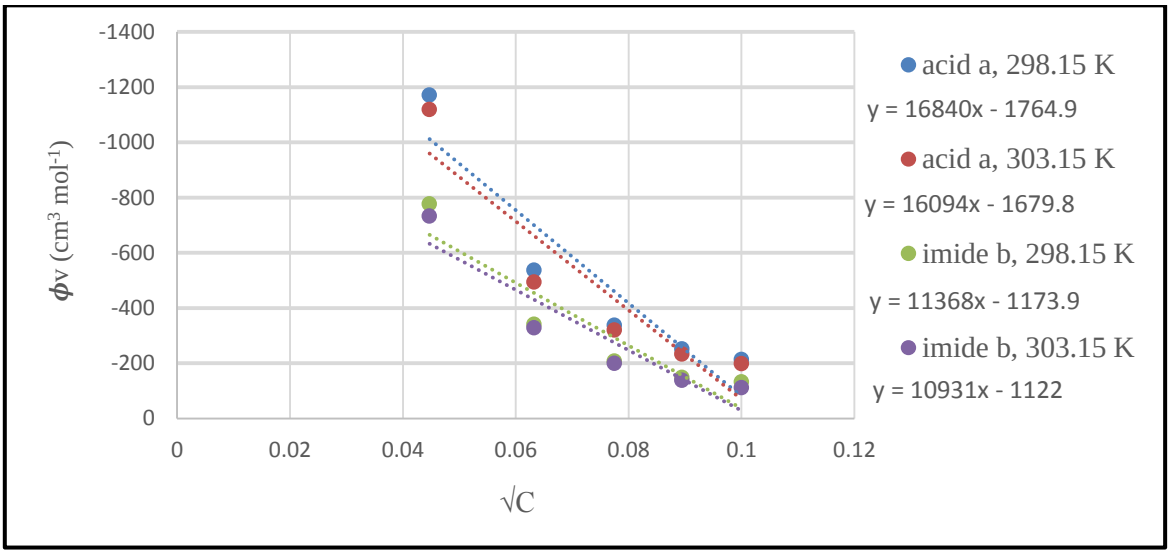

FIGURE 1: Plot of ϕ_v vs c½ of N-phenyl maleanilic acid and N-phenyl maleimide in aqueous dimethyl sulphoxide at 298.15 and 303.15 K.

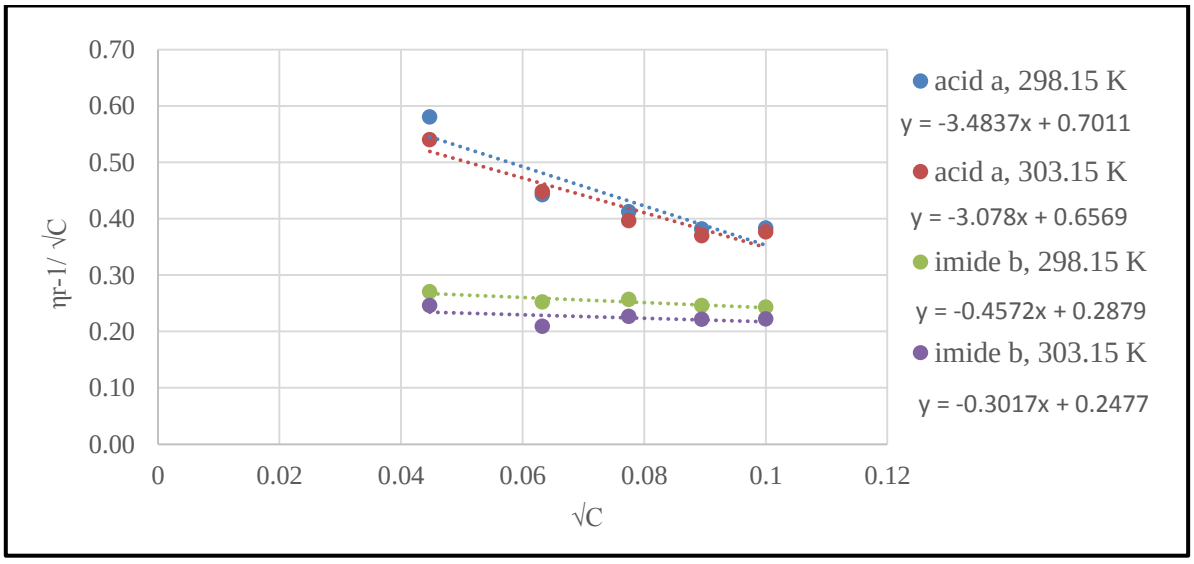

FIGURE 2: Plot of $(\eta_r-1)/c^{½}$ vs $c^{½}$ of N-phenyl maleanilic acid and N-phenyl maleimide in aqueous dimethyl sulphoxide at 298.15 and 303.15 K.

TABLE 2: Masson and Jones-Dole Parameters of N-phenyl maleanilic acid (a) and N-phenyl maleimide (b) in aqueous dimethyl sulphoxide at 298.15 and 303.15 K.

Comp.	ϕo_v	S_v	A ($dm^{3/2}mole^{-1/2}$)	B (dm^3mole^{-1})
298.15 K				
a	-1764.9	16840	0.7011	-3.484
b	-1173.9	11368	0.288	-0.457
303.15 K				
a	-1679.8	16094	0.6569	-3.078
b	-1122.0	10931	0.248	-0.302

Conclusion:

In the present work we have systematically reported molecular interaction study of N-phenyl maleanilic acid (a) and maleimide (b) in aqueous dimethyl sulphoxide solution at 298.15 and 303.15 K. It was observed that negative the values of apparent molar volume indicate strong molecular association in compound a and b. Positive values of Sv and viscosity constant 'A' indicate the presence of strong solute-solute interaction that becomes weak with rise in temperature. The extent of interactions were found to be more in N-phenyl maleanilic acid than the N-phenyl maleimide. The value of Jones-Dole coefficient 'B' indicates strong interactions between solute and solvent at higher temperature. The Jones -Dole and Masson's equations were found to be obeyed for maleanilic acid and maleimide in 80 % aqueous dimethyl sulphoxide solution at 298.15 and 303.15 K.

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